Phase Diagrams of $S = 3/2, 2$ XXZ Spin Chains with Bond-Alternation

Atsuhiro Kitazawa[1,2] and Kiyohide Nomura[1]

[1]*Department of Physics, Kyushu University, Fukuoka 812-12, Japan*

[2]*Department of Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152,*

Japan

(February 1, 2008)

Abstract

We study the phase diagram of $S = 3/2$ and $S = 2$ bond-alternating spin chains numerically. In previous papers, the phase diagram of $S = 1$ XXZ spin chain with bond-alternation was shown to reflect the hidden $Z_2 \times Z_2$ symmetry. But for the higher S Heisenberg spin chain, the successive dimerization transition occurs, and for anisotropic spin chains the phase structure will be more colorful than the $S = 1$ case. Using recently developed methods, we show directly that the phase structure of the anisotropic spin chains relates to the $Z_2 \times Z_2$ symmetry.

Haldane predicted that the antiferromagnetic Heisenberg spin chain has different behaviors between integer and half odd integer spins [1]. For half odd integer spin cases, the ground state has gapless excitations and spin correlations decay in the power law. The ground state properties for half odd spin Heisenberg chains are the same ones of the $S = 1/2$ case. On the other hand for integer spin cases, the ground state is a singlet with finite excitation gap and the spin correlations decay exponentially. Another aspect for the Haldane gapped state was presented by Affleck *et.al.* [2]. They studied a special $S = 1$ $SU(2)$ spin chain which has the property of the Haldane gap conjecture, and proposed valence bond solid (VBS) states. The $S = 1$ VBS state has the hidden antiferromagnetic structure. Later den Nijs and Rommelse [3] found the string order parameter as the order parameter for it.

Using a non-local unitary transformation, Kennedy and Tasaki [4] showed that the broken symmetry of $S = 1$ Haldane gap systems is a $Z_2 \times Z_2$ type. Nearly four-fold degenerate states of the system with open boundary conditions reflect the discrete symmetry. For the higher S cases, Oshikawa [5] showed that odd integer S VBS states break the hidden $Z_2 \times Z_2$ symmetry, while even integer S VBS states do not violate the hidden $Z_2 \times Z_2$ symmetry, and considered the generalized string order parameters. He pointed out another possibilities for the broken symmetry of higher S cases.

In our previous papers with Okamoto [6,7], we studied the $S = 1$ XXZ spin chains with the bond-alternation,

$$H = \sum_{j=1}^{N} \left[1 - (-1)^j \delta\right] \left[S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z\right] \tag{1}$$

and we obtained the phase diagram reflecting the hidden $Z_2 \times Z_2$ symmetry. Comparing with the phase structure of the quantum Ashkin-Teller model [8] which has a $Z_2 \times Z_2$ symmetry explicitly, the possible phase diagram consists of the two dimensional(2D) Ising, the Gaussian, and the Berezinskii-Kosterlitz-Thouless(BKT) transitions. Combining the quantum Ashkin-Teller picture with the generalized hidden $Z_2 \times Z_2$ symmetry, we predicted that for $-1 < \Delta$, $-1 < \delta < 1$, there are $2S + 1$ 2D Ising, $2S$ Gaussian, and $2S + 1$ BKT critical lines. Especially the Gaussian lines should separate several VBS states, as was argued

by Guo *et.al.* [9] and Oshikawa [5]. According to them, the VBS state with the periodic boundary condition can be written by

$$|S, M, \text{PBC}\rangle$$
$$= (a_N^\dagger b_1^\dagger - b_N^\dagger a_1^\dagger)^{S-M} \times$$
$$\prod_{j=1}^{N/2-1} (a_{2j-1}^\dagger b_{2j}^\dagger - b_{2j-1}^\dagger a_{2j}^\dagger)^{S+M} (a_{2j}^\dagger b_{2j+1}^\dagger - b_{2j}^\dagger a_{2j+1}^\dagger)^{S-M}$$
$$\times (a_{N-1}^\dagger b_N^\dagger - b_{N-1}^\dagger a_N^\dagger)^{S+M} |0\rangle, \tag{2}$$

where we describe the spin state by the Schwinger bosons, that is, $a_j^\dagger(b_j^\dagger)$ creates the $S = 1/2$ $\uparrow (\downarrow)$ state at the j-th site, and M is an integer for integer S, or a half integer for half integer S, which changes from $-S$ to S if we vary δ from -1 to 1. Hereafter we denote this VBS state as M-VBS state. Oshikawa [5] showed that for integer S case, the hidden $Z_2 \times Z_2$ symmetry is broken in the M-VBS state when $S-M$ is an odd integer. For the isotropic case $(\Delta = 1)$, the $S = 1$ case is known that the transition between the Haldane and the dimer phases occurs about $\delta = 0.26$ [10–13,7]. For the $S = 3/2$ case, Yajima and Takahashi [14] studied with the density matrix renormalization group method and evaluated the transition point between $M = 1/2$ and $M = 3/2$ phase as $\delta_{1/2-3/2} = 0.42 \pm 0.02$. Yamamoto [13] obatained consistent results as $\delta_{1/2-3/2} = 0.43 \pm 0.01$ by quantum Monte Calro calculation. For the $S = 2$ case, Yamanaka, Oshikawa, and Miyashita [15] evaluated the transition point by quantum Monte Carlo calculation. They obtained that the transition point between $M = 0$ and $M = 1$ phases is in the region $0.05 < \delta_{0-1} < 0.3$, and the transition point between $M = 1$ and $M = 2$ is in the region $0.5 < \delta_{1-2} < 0.6$. Yamamoto [13] evaluated the transition point of $S = 2$ case more accurately as $\delta_{0-1} = 0.18 \pm 0.01$, $\delta_{1-2} = 0.545 \pm 0.005$.

In this paper, we show the phase diagram of the model(1) for $S = 3/2$ and $S = 2$ cases with the exact diagonalization method for finite size systems. In the following, we mainly argue the successive dimerization of the model(1).

We use the following sine-Gordon Euclidean action as an effective model [16] of the Hamiltonian(1)

$$S = \frac{1}{2\pi} \int v d\tau dx \frac{1}{K} \left[\left(\frac{\partial \phi}{v \partial \tau} \right) + \left(\frac{\partial \phi}{\partial x} \right) \right] \tag{3}$$
$$+ \frac{y_1}{2\pi a^2} \int v d\tau dx \cos \sqrt{2}\phi + \frac{y_2}{2\pi a^2} \int v d\tau dx \cos \sqrt{8}\phi,$$

where a is a lattice constat and v is the sound velocity. The dual field θ is defined as

$$\frac{\partial}{v \partial \tau} \phi(\tau, x) = -\frac{\partial}{\partial x}(iK\theta(\tau, x)),$$
$$\frac{\partial}{\partial x} \phi(\tau, x) = \frac{\partial}{v \partial \tau}(iK\theta(\tau, x)).$$

We make the identification $\phi \equiv \phi + \sqrt{2}\pi$, $\theta \equiv \theta + \sqrt{2}\pi$. For the free field theory, the primary operators $\exp(in\sqrt{2}\theta + im\sqrt{2}\phi)$ have the scaling dimension $x_{n,m} = n^2/2K + m^2 K/2$ and the spin $s_{n,m} = nm$ (where integer variables n and m are electric and magnetic charges in the Coulomb gas picture). The second term of eq.(3) is the mass term for the Haldane gap systems [16,17]. (According to Affleck [17], we have $y_1 \propto \cos \Theta/2$, where Θ is the topological angle.)

After scaling $a \to ae^{dl}$, we obtain the following 1-loop renormalization group equations

$$\frac{d}{dl}\frac{1}{K} = \frac{1}{8}y_1^2 + \frac{1}{2}y_2^2,$$
$$\frac{dy_1}{dl} = \left(2 - \frac{K}{2}\right)y_1 - \frac{1}{2}y_1 y_2, \tag{4}$$
$$\frac{dy_2}{dl} = (2 - 2K)y_2 - \frac{1}{4}y_1^2.$$

From these equations we can neglect the third term of eq.(3) for $K > 1$. The third term is important for the 2-D Ising transition and the level-1 $SU(2)$ WZW point, but not for the BKT and the Gaussian transitions. Neglecting y_2 we obtain the following Kosterlitz's recursion relation

$$\frac{d}{dl}\frac{1}{K} = \frac{1}{8}y_1^2, \quad \frac{dy_1}{dl} = \left(2 - \frac{K}{2}\right)y_1. \tag{5}$$

Near $K = 4$, there occurs the BKT transition, and for $4 > K > 1$ the Gaussian transition occurs at $y_1 = 0$.

The obtained phase diagrams are in Fig.1 for $S = 3/2$ case and in Fig.2 for $S = 2$ case using the method in [19,20]. The topology of the phase diagrams is consistent with the prediction as is described above.

At this stage, we will explain the method to determine the Gaussian line and the relation to the $Z_2 \times Z_2$ symmetry. Considering the hidden $Z_2 \times Z_2$ symmetry, the successive dimerized transitions are of the Gaussian type. The Hamiltonian is invariant under the space inversion $P{:}j \to N - 1 + j$ and the spin reversal $T{:}a^\dagger \leftrightarrow b^\dagger$ and all states(2) have the same eigenvalues of P and T ($P = T = (-1)^{SN}$, independent of M). For the transition from M phase to the $M + 1$ one, the ground state is singlet in both phases, so we can not simply apply the phenomenological renormalization group technique. But with the twisted boundary condition

$$S_{N+1}^x \pm iS_{N+1}^y = -(S_1^x \pm iS_1^y), \quad S_{N+1}^z = S_1^z,$$

the M-VBS state(2) changes to [7]

$$
\begin{aligned}
&|S, M, \text{TBC}\rangle \\
&= (a_N^\dagger b_1^\dagger + b_N^\dagger a_1^\dagger)^{S-M} \times \\
&\prod_{j=1}^{N/2-1} (a_{2j-1}^\dagger b_{2j}^\dagger - b_{2j-1}^\dagger a_{2j}^\dagger)^{S+M}(a_{2j}^\dagger b_{2j+1}^\dagger - b_{2j}^\dagger a_{2j+1}^\dagger)^{S-M} \\
&\times (a_{N-1}^\dagger b_N^\dagger - b_{N-1}^\dagger a_N^\dagger)^{S+M}|0\rangle.
\end{aligned} \tag{6}
$$

From this equation, the M-VBS state has $P = T = (-1)^{SN-S+M}$ and the $M + 1$ state has $P = T = (-1)^{SN-S+M+1}$, so the two states have the different symmetries, and the energy levels cross at the transition point.

In the sine-Gordon Language, the effect of the twisted boundary condition is to shift the magnetic charge m as $m \to m + 1/2$ [18], so only the half integer magnetic charge operators exist. Then we have the following size dependence of the scaling dimensions of the $m = \pm 1/2$ operators $\sqrt{2}\cos(\phi/\sqrt{2})$ $[x_{0,1/2}^e]$ and $\sqrt{2}\sin(\phi/\sqrt{2})$ $[x_{0,1/2}^o]$ [19],

$$
\begin{aligned}
x_{0,1/2}^e(L) &= \frac{L(E_{L,\pi}^e - E_{L,0}^e)}{2\pi v} = \frac{K}{8} + \frac{y_1(L)}{2} + \cdots, \\
x_{0,1/2}^o(L) &= \frac{L(E_{L,\pi}^o - E_{L,0}^e)}{2\pi v} = \frac{K}{8} - \frac{y_1(L)}{2} + \cdots,
\end{aligned}
$$

where L is the system size, y_1 is a renormalized function of L as

$$y_1(L) = y_1 \left(\frac{2\pi}{L}\right)^{K/2-2},$$

$E_{L,0}^e$ is the ground state energy of the periodic boundary conditions, and we denote $E_{L,\pi}^{e;o}$ as the corresponding energy to $\sqrt{2}\cos(\phi/\sqrt{2})$, $\sqrt{2}\sin(\phi/\sqrt{2})$ (e,o mean the parity $P = 1$, -1). In this method, the correction from the third term of eq.(3) does not affect since this method uses the duality of the quantum Ashkin-Teller model [7]. Note that Kolb [21] studied the XXZ spin chain with the twisted boundary condition $S_{N+1}^\pm = e^{\pm i\Phi}S_1^\pm$, $S_{N+1}^z = S_1^z$ and showed that for the half integer spin model the ground states are two-fold degenerate at $\Phi = \pi$, since for the half integer S XXZ spin chains, the second term in eq.(3) is absent ($y_1 = 0$).

For $S = 3/2$ case, we study the $N = 6, 8, 10, 12$ systems. In Fig. 3, we show the two low lying energies of the subspace $\sum S^z = 0$ with the twisted boundary condition for $\Delta = 1$, $N = 12$. For small $\delta (> 0)$ the lowest state has $P = T = 1$, and for $1 > \delta > \delta_{1/2-3/2}$ the lowest state has $P = T = -1$, as expected from eq.(6). Fig. 4 shows the size dependence of the crossing point. We extrapolated the crossing point as polynomials of $1/N^2$ [7] and the evaluated value is $\delta_{1/2-3/2} = 0.4315$, which is consistent with the previously obtained value [14,13]. For the BKT transitions between the XY and the VBS phases are determined by the similar method in ref [20] (see also [6,7]). The evaluated multi-critical points of the XY, M-VBS, and $M + 1$ VBS phases are $(\Delta_M, \delta_M) = (0.8188, 0)$, $(0.5766, \pm 0.4052)$. For the transitions between the Néel and the VBS phases (2D Ising type), we use the phenomenological renormalization group method.

For $S = 2$ case, we calculate the energy eigenvalues for $N = 4, 6, 8, 10$. In Fig. 5, we show the two low lying energies of the subspace $\sum S^z = 0$ with the twisted boundary condition for $\Delta = 1$, $N = 10$. The level crossing occurs two times for $0 < \delta < 1$. For $0 < \delta < \delta_{0-1}$ the lowest state has $P = T = 1$ ($S = 2$ Haldane phase, $M = 0$), for $\delta_{0-1} < \delta < \delta_{1-2}$ the lowest state has $P = T = -1$ ($M = 1$), and for $\delta_{1-2} < \delta < 1$ the lowest state has $P = T = 1$ ($M = 2$), as expected from eq.(6). The hidden $Z_2 \times Z_2$ symmetry is broken for $M = \pm 1$ phase. Fig. 6 shows the size dependence of the crossing point (δ_{0-1}). The extrapolated

values of the transition points are $\delta_{0-1} = 0.1830$ (between $M = 0$ and $M = 1$ VBS phases), and $\delta_{1-2} = 0.5505$ (between $M = 1$ and $M = 2$ VBS phases). These values are consistent with the results of Yamamoto [13]. For $\delta = 0$, the transition point between the XY and the $S = 2$ Haldane phases is $\Delta_c = 0.9650$. The evaluated multi-critical points between the XY and the VBS phases are $(\Delta_M, \delta_M) = (0.9708, \pm 0.1823)$ and $(0.8401, \pm 0.5325)$.

In this paper, we showed the phase diagrams of the $S = 3/2, 2$ bond-alternating XXZ spin chain. On the base of the hidden $Z_2 \times Z_2$ symmetry, we can see the successive dimerization numerically using the twisted boundary conditions. The two lowest excitations in the twisted boundary condition correspond to the order parameter and its dual disorder parameter (with respect to the $Z_2 \times Z_2$ symmetry) [7], so their crossing point is the self-dual point (in the Ashkin-Teller language) or the Gaussian critical point. Therefore, we can determine the critical point more precisely than the method using the string order parameter only [12], especially near the BKT multicritical point.

REFERENCES

[1] F. D. M. Haldane, Phys. Lett.**93A** 464 (1983); Phys. Rev. Lett. **50** 1153 (1983).

[2] I. Affleck, T. Kennedy, E. Leib, and H. Tasaki, Phys. Rev. Lett. **59** 799 (1987); Commun. Math. Phys. **115** 477 (1988).

[3] M. den Nijs and K. Rommelse, Phys. Rev. **B40**, 4709 (1989).

[4] T. Kennedy and H. Tasaki, Phys. Rev. **B 45**, 304 (1992), Commun. Math. Phys. **147**, 431, (1992).

[5] M. Oshikawa, J. Phys.:Condens. Matter **4**, 7469 (1992).

[6] A Kitazawa, K. Nomura, and K Okamoto, Phys. Rev. Lett. **76** 4038 (1996).

[7] A. Kitazawa and K. Nomura, preprint cond-mat/9705179.

[8] M. Kohmoto, M. den Nijs, and L. P. Kadanoff, Phys. Rev. **B 24**, 5229 (1981).

[9] D. Guo. T. Kennedy, and S. Mazumdar, Phys. Rev. **B41** 9592 (1990).

[10] Y. Kato and A. Tanaka, J. Phys. Soc. Jpn. **63**,1277 (1994).

[11] S. Yamamoto, J. Phys. Soc. Jpn. **63**,4327 (1994); Phys. Rev. B **51**, 16128 (1995).

[12] K. Totsuka, Y. Nishiyama, N. Hatano, and M. Suzuki, J. Phys. Condens. Matter **7**, 4895 (1995).

[13] S. Yamamoto, Phys. Rev. B **55** 3603 (1997).

[14] M. Yajima and M. Takahashi, J. Phys. Soc Jpn **65**, 39 (1996).

[15] M. Yamanaka, M. Oshikawa, and S. Miyashita, J. Phys. Soc Jpn **65**, 1562 (1996).

[16] H. J. Schulz, Phys. Rev. B **34**, 6372 (1986).

[17] I. Affleck, Phys. Rev. Lett. **56**, 408 (1986).

[18] F. C. Alcaraz, M. N. Barber, and M. T. Batchelor, Ann. Phys. (N.Y.) **182**, 208 (1988).

[19] A. Kitazawa, J. Phys. A **30**, L285 (1997).

[20] K. Nomura, J. Phys.**A 28**, 5451 (1995).

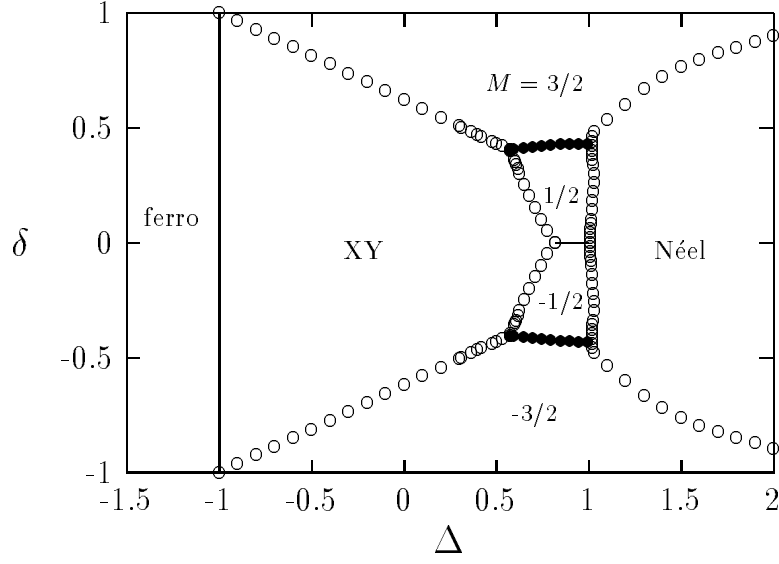[21] M. Kolb, Phys. Rev. B **31**, 7494 (1985).

FIG. 1. Phase diagram of the $S = 3/2$ model. The solid circles and the horizontal line separate $M = -3/2, -1/2, 1/2, 3/2$ VBS phases. Transitions between the XY and the VBS phases are of the BKT type. Transitions between the Néel and the VBS phases are of the 2D Ising type.
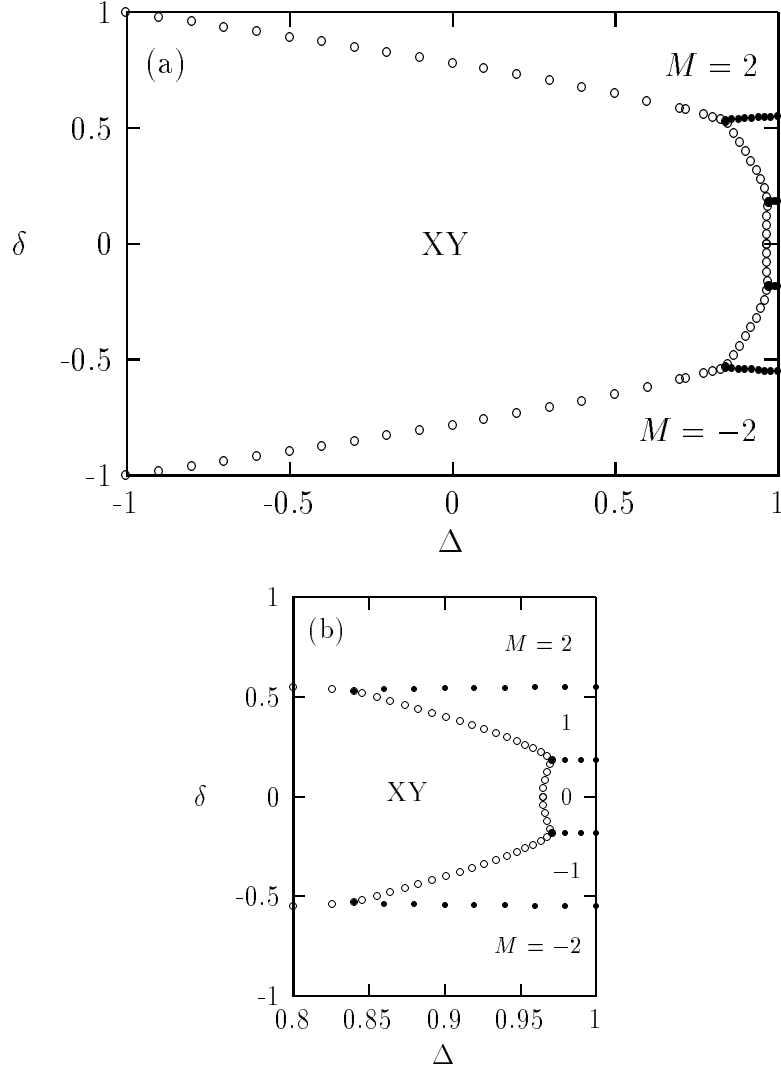
FIG. 2. Phase diagram of the $S = 2$ model in the region (a):$-1 < \Delta < 1$, and (b):$0.8 < \Delta < 1$. Solid circles separate $M = -2, -1, 0, 1, 2$ VBS phases.
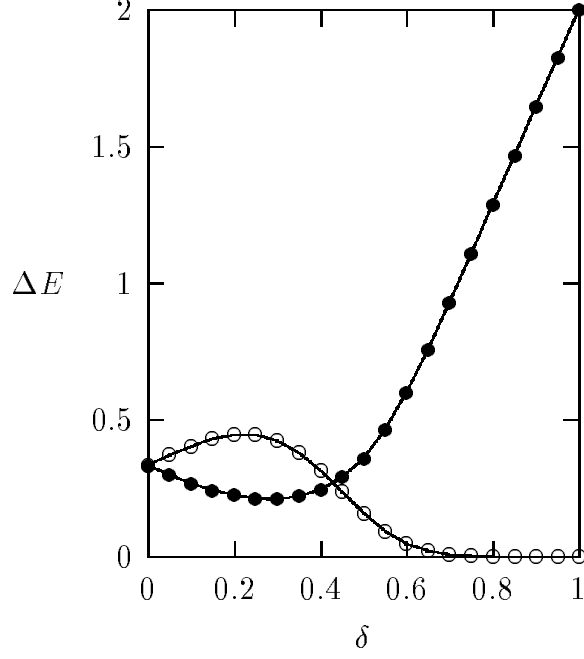
FIG. 3. $E_{N,\pi}^e - E_{N,0}^e$ ($P = T = 1$) ($\circ$) and $E_{N,\pi}^o - E_{N,0}^e$ ($P = T = -1$) ($\bullet$) of $S = 3/2$, $\Delta = 1$, $N = 12$ systems.
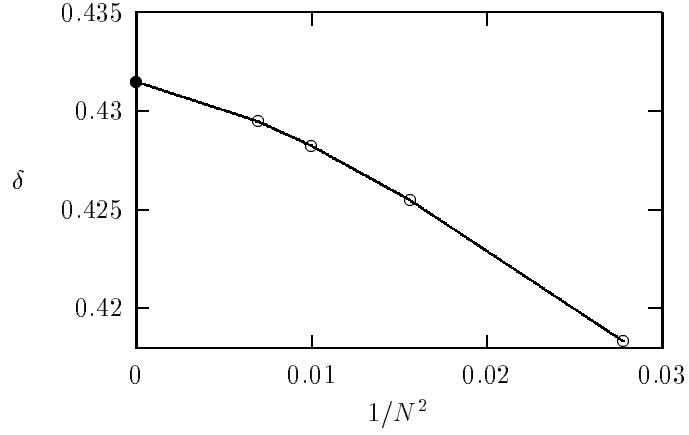

FIG. 4. Size dependence of the crossing points ($\delta_{1/2-3/2}$) for $S = 3/2$ and $\Delta = 1$.
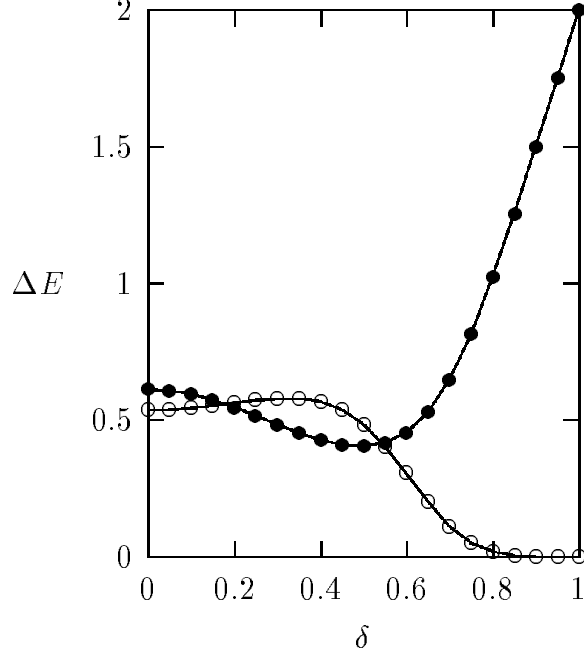
FIG. 5. $E_{N,\pi}^e - E_{N,0}^e$ ($P = T = 1$) ($\circ$) and $E_{N,\pi}^o - E_{N,0}^e$ ($P = T = -1$) ($\bullet$) of $S = 2$, $\Delta = 1$, $N = 10$ systems.
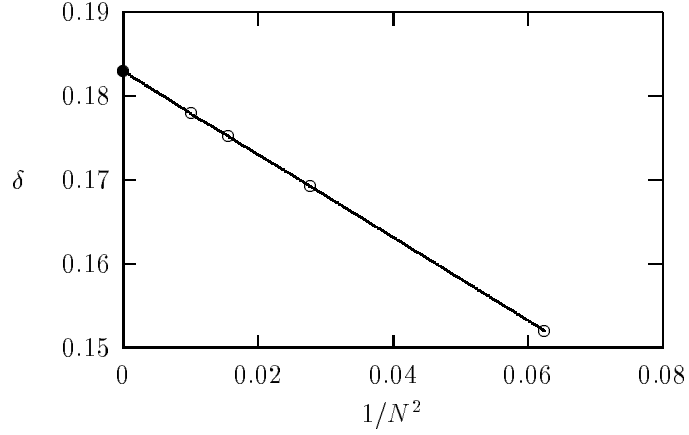

FIG. 6. Size dependence of the crossing points (δ_{0-1}) for $S = 2$ and $\Delta = 1$.